

June 2018

Science & Technology

REVIEW

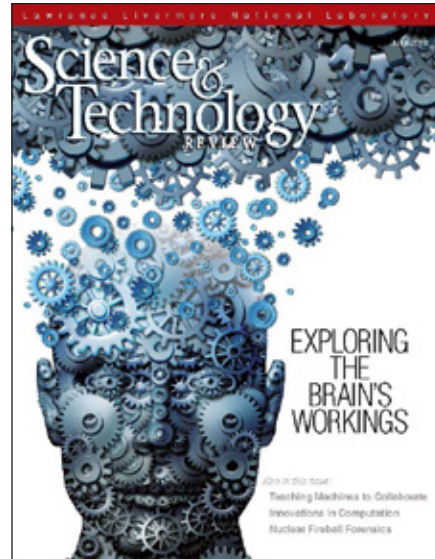
EXPLORING THE BRAIN'S WORKINGS

Also in this issue:

Teaching Machines to Collaborate
Innovations in Computation
Nuclear Fireball Forensics

About the Cover

Lawrence Livermore's Neurotechnology Program is designing and building extremely small, biocompatible devices called microelectrode arrays that can be implanted in the brain. These arrays, called Livermore Flexible Probes, monitor and optionally stimulate neural activity. As the article beginning on p. 4 describes, research laboratories across the nation are now using Livermore Flexible Probes for recording neural activity in the brains of humans and animals. Researchers are hopeful the vast amounts of data collected from the arrays will point the way to innovative treatments for both neurological disorders and neuropsychiatric conditions, including depression and post-traumatic stress disorder.



Cover design: Mark Gartland

About S&TR

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published eight times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

The Laboratory is operated by Lawrence Livermore National Security, LLC (LLNS), for the Department of Energy's National Nuclear Security Administration. LLNS is a partnership involving Bechtel National, University of California, Babcock & Wilcox, Washington Division of URS Corporation, and Battelle in affiliation with the Texas A&M University. More information about LLNS is available online at www.llnslc.com.

Please address any correspondence (including name and address changes) to *S&TR*, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 423-3432. Our e-mail address is str-mail@llnl.gov. *S&TR* is available on the Web at str.llnl.gov.

© 2018. Lawrence Livermore National Security, LLC. All rights reserved. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. To request permission to use any material contained in this document, please submit your request in writing to Public Affairs Office, Lawrence Livermore National Laboratory, Mail Stop L-3, P.O. Box 808, Livermore, California 94551, or to our e-mail address str-mail@llnl.gov.

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.

S&TR Staff

SCIENTIFIC EDITOR
Kathryn M. Mohr

MANAGING EDITOR
Ken Chinn

PUBLICATION EDITOR
Paul Kotta

WRITERS
Lauren Casonhua, Allan Chen,
Arnie Heller, Ben Kennedy,
and Dan Linehan

ART DIRECTOR
Mark Gartland

DESIGNER
Amy Henke

PROOFREADER
Caryn Meissner

S&TR ONLINE
Lauren Casonhua, Rose Hansen,
Lanie L. Helms, and Pam Davis Williams

PRINT COORDINATOR
Diana Horne

S&TR, a Director's Office publication, is produced by the Technical Information Department under the direction of the Office of Planning and Special Studies.

S&TR is available on the Web
at str.llnl.gov

Printed in the United States of America

Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22161

UCRL-TR-52000-18-6
Distribution Category UC-99
June 2018

Science & Technology REVIEW

June 2018

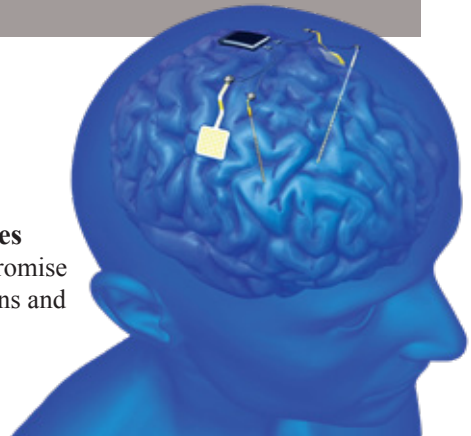
Lawrence
Livermore
National
Laboratory

Contents

Feature

3 Advancing the Frontiers of Neuroscience and Neurotechnology
Commentary by Anantha Krishnan

4 Delving Deeply into the Brain's Mysteries
Tiny biocompatible microelectrode implants promise greater understanding of how the brain functions and new treatments for neurological disorders.



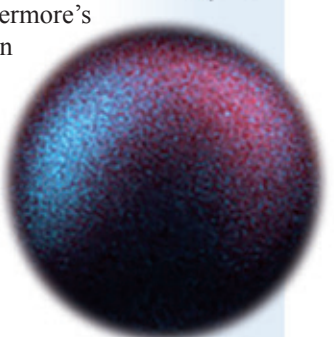
Research Highlights

12 Building a Network of Collaborative Autonomous Machines
Imbuing a system of mobile, networked platforms with distributed intelligence and decision-making capability is the next cybernetic frontier.



16 Grassroots Innovation Grows Great Computational Ideas
Harnessing more than just computing power, Lawrence Livermore's Computation directorate is taking advantage of collaboration and creativity across the entire Laboratory.

20 Piecing Together a Nuclear Fireball
By studying how different elements react inside a nuclear fireball, researchers gain valuable insight into predetonation conditions.



Departments

2 The Laboratory in the News

24 Patents and Awards

25 Abstract



Prepared by LLNL under contract
DE-AC52-07NA27344

Accelerating Cancer Drug Discovery

Lawrence Livermore, the Frederick National Laboratory for Cancer Research (FNLCR), GlaxoSmithKline (GSK), and the University of California at San Francisco (UCSF) recently launched a consortium to speed the discovery of effective cancer therapies. Known as Accelerating Therapeutics for Opportunities in Medicine (ATOM), the consortium strives to reduce the time from identified drug target to clinical candidate from approximately 6 years to 12 months.

To achieve this goal, ATOM will develop, test, and validate a multidisciplinary approach to drug discovery in which supercomputing simulations, data science, artificial intelligence, and other cutting-edge know-how are highly integrated into a single drug discovery platform that can ultimately be shared with the entire drug development community. The team will combine chemical and biological screening data provided by GSK with publicly available data and that of future consortium members to generate new dynamic models that can better predict how molecules will behave in the body. Livermore will contribute its supercomputing capabilities, including the next-generation system Sierra, while FNLCR will contribute scientific expertise in precision oncology, computational chemistry, and cancer biology, as well as support for the open sharing of data sets and predictive modeling and simulation tools. UCSF will provide its expertise in drug discovery and medicine to improve the lives of patients.

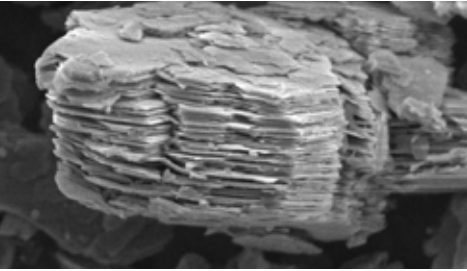
In addition to accelerating cancer drug discovery, ATOM will drive technologies vital to the core missions of the Department of Energy and National Nuclear Security Administration. Livermore Director William Goldstein says, “ATOM will help to strengthen U.S. leadership in high-performance computing and, by speeding the discovery of therapeutics, contribute to biosecurity.”

Contact: Jim Brase (925) 422-6992 (brase1@llnl.gov)

Mineral Waters Earth’s Mantle

The first observation of a super-hydrated phase of the clay mineral kaolinite (see image at right) could improve understanding of processes that lead to volcanism and affect earthquakes. Lawrence Livermore scientist Hyunchoe Cynn and colleagues from Yonsei University in the Republic of Korea, Deutsches Elektronen-Synchrotron in Germany, the Carnegie Institution for Science, George Washington University, SLAC National Accelerator Laboratory, and the University of South Carolina collaborated to re-create subduction zones, where conditions promote formation of the super-hydrated phase of kaolinite. The findings were published online in the November 20, 2017, edition of *Nature Geoscience*.

Subduction zones occur where an oceanic plate dives under the continental crust and plunges into Earth’s mantle. Water



thereby enters the Earth trapped in minerals of the oceanic crust or overlaying sediments, and these minerals slowly sink deeper into the mantle over millions of years. Eventually, the minerals become unstable and transform into new compounds, releasing water that decreases the melting temperature of the mantle rock. “When the mantle rocks melt, magma is generated, leading to volcanic activity when the magma rises to the surface,” says Yongjae Lee from Yonsei University, who led the study.

By re-creating subduction zones in the laboratory, scientists are able to use high-pressure and high-temperature measurements to observe these processes more closely and gain insight into the formation of important oceanic minerals, such as super-hydrated kaolinite. The formation and breakdown of this mineral bears important information about the processes that occur in subduction zones and could help scientists better understand geochemical processes, such as volcanism, in these zones.

Contact: Hyunchoe Cynn (925) 422-3432 (cynn1@llnl.gov).

Global Impact of Arctic Sea Ice Loss

A new study by Ivana Cvijanovic and colleagues from Lawrence Livermore and the University of California at Berkeley shows that substantial loss of Arctic sea ice could have significant worldwide impact, including affecting the amount of precipitation in California. The research appears in the December 5, 2017, online edition of *Nature Communications*.

The team found that sea ice changes can alter convection over the tropical Pacific, thereby driving the formation of an atmospheric ridge in the North Pacific. A phenomenon that played a central role in the 2012–2016 California drought, the atmospheric ridge is known for steering precipitation-rich storms northward, away from California. Although the study does not attribute the 2012–2016 California drought to Arctic sea ice loss, simulations indicate that the sea ice–driven precipitation changes track global rainfall patterns observed during that drought, suggesting that the loss of Arctic sea ice could have played a role.

“The recent California drought appears to be a good illustration of what a sea ice–driven precipitation decline could look like,” says Cvijanovic. Several studies suggest that recent Californian droughts have a human-made component involving increased temperatures, with the likelihood

of such warming-enhanced droughts expected to increase in the future. Cvijanovic says, “Although more research is needed, we should be aware that an increasing number of studies, including this one, suggest that the loss of Arctic sea ice cover is not only a problem for remote Arctic communities but could also affect millions of people worldwide.”

Contact: Ivana Cvijanovic (925) 424-5263 (cvijanovic1@llnl.gov).



Advancing the Frontiers of Neuroscience and Neurotechnology

LAWRENCE Livermore National Laboratory has a long and distinguished history of working at the intersection of engineering and biology in support of national security and human health. Early accomplishments at the Laboratory included chromosome biomarkers, high-speed cell-sorting systems, and instruments for fast polymerase chain reaction. In the late 1990s, the Department of Energy (DOE) established the Chemical and Biological Weapons Nonproliferation Program, and Livermore engineers and bioscientists designed, developed, and prototyped systems to rapidly detect and diagnose a biological attack.

Laboratory researchers have continued to strengthen their expertise in biological science and engineering and micro- and nanotechnology for applications beyond biodetection. In the early 2000s, Livermore was part of a DOE effort to develop the world’s first retinal prosthesis for individuals blinded by end-stage retinitis pigmentosa. The Livermore team developed and prototyped a flexible, highly biocompatible thin-film microelectrode array and a miniaturized, biocompatible, hermetic package containing electronics for stimulating the retina with wireless power. Following successful clinical trials, this technology resulted in a commercial device, the Argus Retinal Prosthesis II, which was approved by the U.S. Food and Drug Administration (FDA) for human use.

As the article beginning on p. 4 describes, Livermore researchers built on the retinal prosthesis legacy in collaboration with clinical partners to develop a number of novel implantable device technologies that can diagnose and potentially treat a multitude of neural disorders. This is exemplified in the Laboratory’s current work on the development of a sense-and-treat—that is, closed-loop and autonomous—neuromodulation system that can access and address any part of the brain, providing unprecedented capability to neurosurgeons and neurologists.

More than 12 million people in the U.S. suffer from some form of serious neuropsychiatric illness—such as depression, anxiety, bipolar disorder, or schizophrenia—or disorders resulting from post-traumatic stress disorder or traumatic brain injury (TBI). Research is starting to show that these debilitating illnesses can be characterized and treated by targeting underlying specific and quantitative evaluations of dysfunctions in brain circuitry rather than subjective clinical assessments.

Deep expertise in novel biocompatible materials and state-of-the-art micro- and nanofabrication, together with advanced signal processing, computational simulation, statistical modeling, and big

data analytics—all combined in a single location—give Lawrence Livermore a unique capability for studying and understanding these disorders. A dedicated fabrication and prototyping facility combines new investments of about \$100 million with decades of expertise in polymer manufacturing and packaging. The Laboratory has successfully manufactured Class III implantable devices in this facility under a quality control system that can support investigational human use with the appropriate FDA approvals. In short, we have created a truly one-of-a-kind research facility to drive fundamental advances in design, development, and early clinical demonstration of implantable devices. By accurately recording brain signals in animals and humans for very long periods of time, these devices are helping to achieve a better understanding of how neurons encode, store, and retrieve information.

At the same time, Livermore researchers are continuing development of the revolutionary iChip (in vitro chip-based human investigational platform) to predict the effects of potentially harmful chemicals, viruses, and drugs on humans without resorting to animal or human test subjects. One variant is a multicellular neurovascular unit that combines brain-on-a-chip technology with an artificial blood–brain barrier to simulate the central nervous system, thereby helping scientists understand how neurons interact with and respond to chemicals. In addition, the Laboratory has partnered with medical groups nationwide to develop an understanding of the mechanisms behind chronic traumatic encephalopathy and, by leveraging the Laboratory’s unique high-performance computing capabilities, to develop improved predictive analytics for the precise diagnosis and treatment of TBI patients.

Current research thrusts are supported by a range of sponsors that include DOE; the Defense Advanced Research Projects Agency; the National Institutes of Health, through the Brain Research through Advancing Innovative Neurotechnologies Initiative; the University of California (UC), through the UC Office of the President Lab-Fee Program; and Livermore’s own Laboratory Directed Research and Development Program. Livermore is also collaborating with several leading academic institutions and private sector partners.

Today, we continue to advance human health by leveraging the Laboratory’s expertise in a truly interdisciplinary fashion. We have a tremendous opportunity to apply our know-how and extraordinary facilities to change the nation’s health care landscape.

■ Anantha Krishnan is associate director for Engineering.



DELVING DEEPLY INTO

S&TR June 2018

Neural Technology

THE BRAIN'S MYSTERIES

Biocompatible microelectrode arrays interface with the brain, promising greater understanding of brain function and new treatments for neurological disorders.

UNDERSTANDING the brain, especially that of humans, is one of the most complex challenges in science today. With an estimated 100 billion neurons joined together by 100 trillion connections in a hugely interconnected network of circuits, the human brain is extraordinarily formidable to investigate. For instance, a brain circuit can encompass not just a group of neighboring neurons but also individual neurons located as far as centimeters away.

Researchers in Lawrence Livermore's Neurotechnology Program, part of the Laboratory's Center for Bioengineering, are responding to the need for innovative approaches to further understanding of brain function and neural communication dynamics. The group is focused on designing and building extremely small and biocompatible devices called Livermore Flexible Probes—microelectrode arrays that are implanted directly into the brain. Also known generically as neural interfaces, Livermore Flexible Probes monitor and optionally stimulate neural activity. Soft and flexible, the probes do not interfere with normal functions or behavior, allowing for long-term studies of brain

circuitry. In animal studies, the probes are already proving to be exceptionally stable and useful.

In fact, research laboratories across the nation are using Livermore Flexible Probes to record neural activity in the brains of both animals and humans. Small-scale animal studies are done at Livermore, while more complex and long-term experiments are being conducted at University of California (UC) campuses and other institutions nationwide with strong neurophysiological

programs. There, researchers test and characterize the mechanical and electrical properties of the implants, as well as their suitability for long-term use. At UC San Francisco (UCSF), the Livermore probes have been successfully tested for short periods on patients undergoing surgery to treat severe epilepsy.

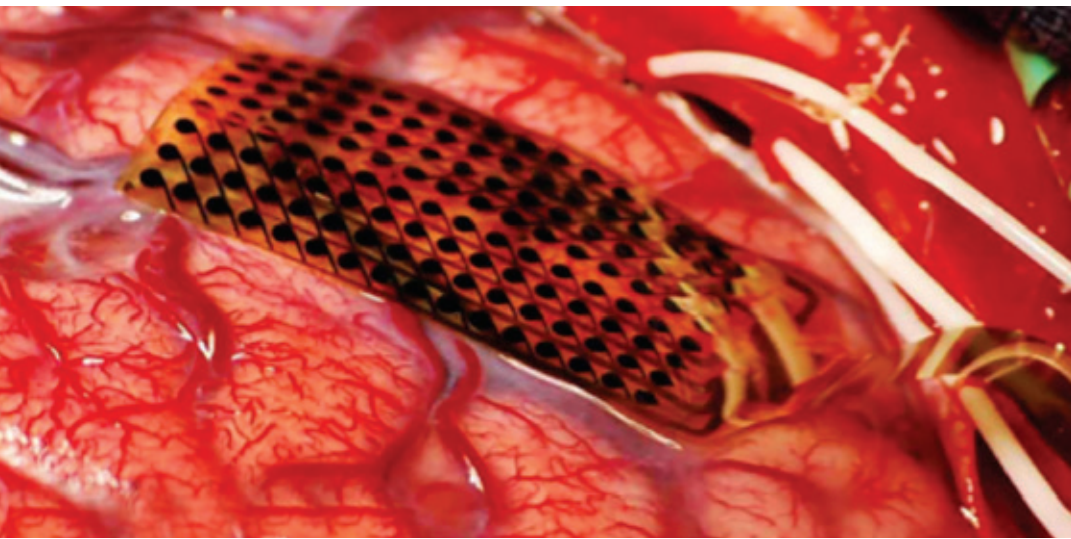
Bolstering a National Effort

Shivshankar Sundaram, director of Livermore's Center for Bioengineering, says, "By providing high-quality,

Livermore's Biomedical Foundry includes a clean room that is recognized nationally as a unique thin-film neural interface facility. Here researchers fabricate components for the Livermore Flexible Probes. (Photo by Randy Wong.)

A researcher holds an example of a Livermore Flexible Probe. The probes are designed to record data on the neural activity of animal and human brains in situ. (Photo by Randy Wong.)





A 128-electrode Livermore Flexible Probe temporarily implanted in the hippocampus of a patient at the University of California at San Francisco. (Photo courtesy of Dr. Eddie Chang.)

long-term, and continuous recordings of brain activity with high resolution, the Livermore work enhances a larger national effort to revolutionize understanding of the brain and uncover ways to diagnose, treat, and prevent brain disorders.” Researchers are hopeful that the vast amounts of data being collected from the arrays will point the way to innovative treatments for both neurological disorders—such as Parkinson’s disease—and neuropsychiatric conditions, such as generalized anxiety, depression, and post-traumatic stress disorder (PTSD). The arrays may even one day restore lost neural functions such as sight, hearing, mobility, and memory.

Lawrence Livermore’s long history of developing innovative bioengineering systems dates back to the 1970s, when researchers developed the first laser-based cell sorters, and continues through the development of miniaturized polymerase chain reaction systems that revolutionized molecular diagnostics. These pioneering achievements took advantage of a core Livermore strength—precisely recording,

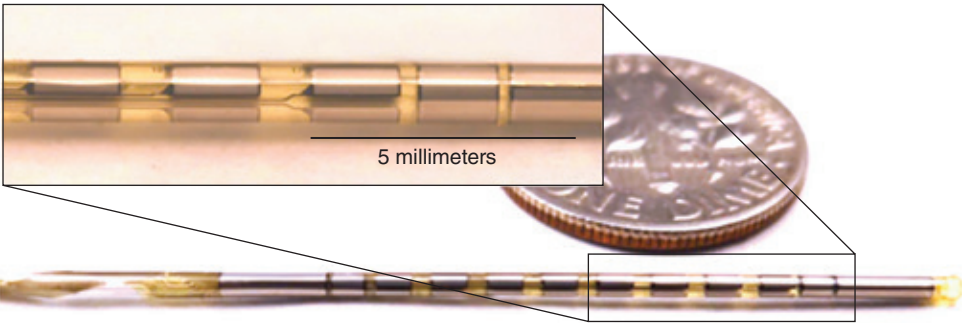
measuring, and analyzing data from complex systems, ranging from air turbulence to inertial confinement fusion reactions—and led to Livermore’s involvement in both fabricating implanted biomedical devices and handling the large amounts of data the devices collect. The neural interface work also underscores the Laboratory’s growing leadership in precision medicine initiatives such as the Accelerating Therapeutics for Opportunities in Medicine Consortium, the national Cancer Moonshot initiative, and human organ models that use three-dimensional bioprinting and microchips to re-create human physiology outside the body.

Much of the foundational research and development on flexible materials for microelectrodes was originally

supported by the Department of Energy’s Retinal Prosthesis Program, with additional support from the National Institutes of Health (NIH), UC’s Office of the President, and Livermore’s own Laboratory Directed Research and Development Program. Current research is funded by the Department of Defense’s Defense Advanced Research Projects Agency (DARPA) and the federal Brain Research through Advancing Innovative Neurotechnologies (BRAIN) Initiative. Launched in 2013, the BRAIN Initiative aims to revolutionize scientific understanding of the human brain by discovering how individual cells and neural circuits interact in both time and space and uncovering ways to treat, prevent, and cure brain disorders and traumatic brain injuries. Participating in the initiative are federal agencies, national laboratories, foundations, universities, institutes, and private industry.

A strong relationship with bioengineers, neuroscientists, and surgeons nationwide is critical to Livermore’s research effort. For example, Livermore’s microfabrication know-how complements clinical science expertise at UCSF. A Livermore–UCSF team developed a method to implant the Livermore Flexible Probes into deep brain tissue with the aid of a removable device.

Although commercial devices commonly feature only 4 electrodes, Livermore designs offer 32, 64, and even 128 electrodes, enabling the capture of more data at higher rates.



At UCSF, the Livermore team works closely with neurosurgeon Eddie Chang and with Loren Frank, who is focused on neural circuits that underlie learning and decision making. Other collaborators include electronics researchers at Lawrence Berkeley National Laboratory and Professor Charles Della Santina at Johns Hopkins University.

Recording at High Density

Acquiring an in-depth understanding of how the brain functions and how signals flow within and between brain regions requires recording signals at high density, in multiple brain regions, and for long durations—up to several months or even years. Researchers need high-density neural interfaces implanted for long periods to understand brain networks. However, most commercial implants are bulky, handmade devices that provide limited resolution and are typically made of rigid and breakable silicon, which can damage brain tissue. Such devices are often quickly rejected by the immune system as foreign objects, making it nearly impossible to take long-term recordings of awake animals. “The body is a harsh environment for electronics,” notes Sundaram. “We can’t simply embed something and not expect the body to attack it as foreign.” Moreover, components must be sealed off from bodily fluids that would cause electronics to short circuit.

Once implanted, Livermore Flexible Probes can last for long periods without their performance degrading. Indeed, animal experiments conducted at several university laboratories are demonstrating that the probes uniformly achieve long-term, high-density recordings from multiple brain regions. One key to this longevity is the thin polymer film that insulates the device and allows it to move naturally with the micromotions of the brain. “Brain tissue is flexible like gelatin, so we need to build devices that match those mechanical properties,”



explains Razi Haque, head of Livermore’s Neurotechnology Program and leader of several projects involving neural implantable probes. Haque says, “The devices’ flexibility allows placement underneath imaging windows without danger of breakage, making possible combined electrophysiology and imaging studies.” The Livermore devices also support optogenetic stimulation, a technique that uses light and light-sensitive proteins to manipulate neural activity.

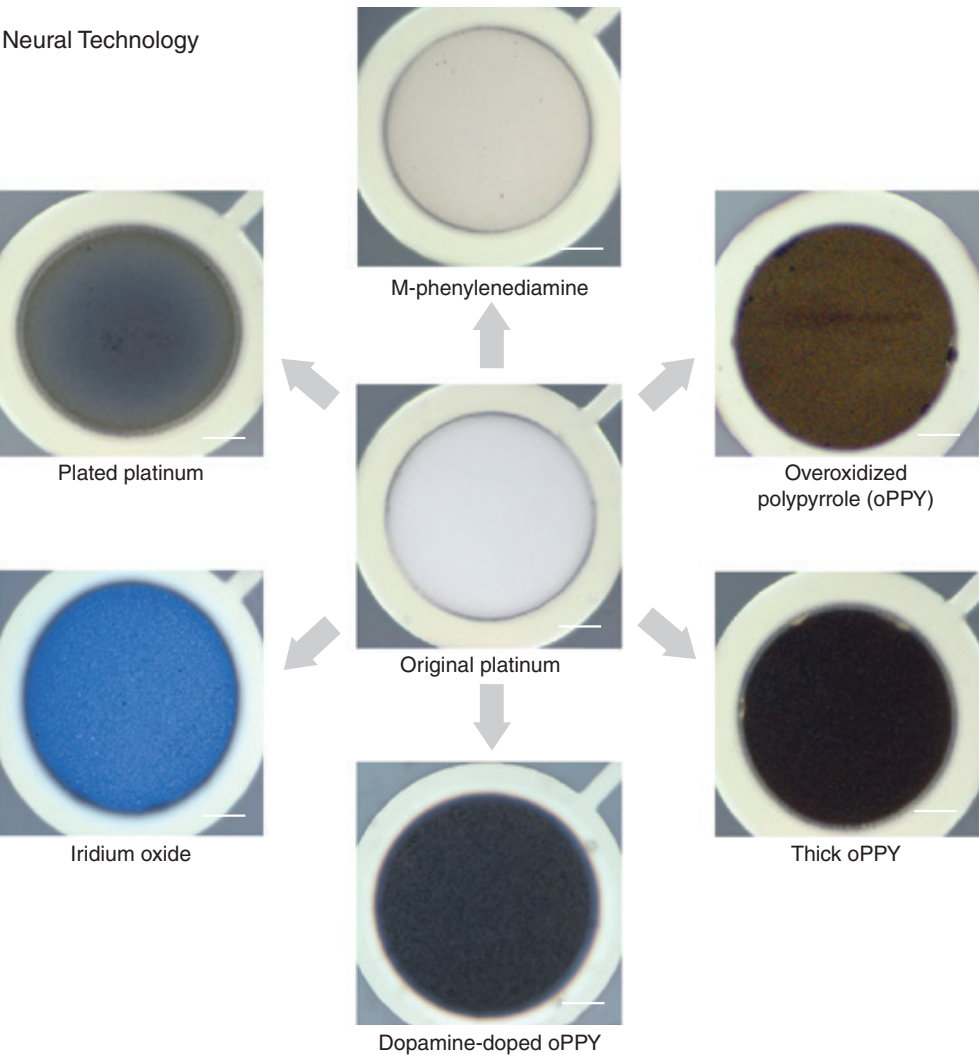
Manufacturing in Clean Rooms

Livermore Flexible Probes are produced with Laboratory microfabrication techniques—many of them patented—at the Biomedical Foundry, in the Laboratory’s Center for Micro- and Nanotechnologies. The foundry includes a clean room with dedicated processing and characterization equipment and is recognized nationally as a unique thin-film neural interface facility. “We have a singular skill set in microfabrication coupled with tight control over manufacturing,” declares Haque. In fact,

A researcher in the clean room holds wafers on which Livermore Flexible Probes electronics have been manufactured. The probes consist of metal layers separated and insulated by flexible, biocompatible polyimide films. Fabrication employs the same photolithographic process that the electronics industry uses to manufacture integrated circuits, building a device layer by layer. (Photo by Randy Wong.)

quality control is key for the Livermore Flexible Probes that has been approved for use in humans. The clean room–produced probes consist of metal layers separated and insulated by flexible, biocompatible polyimide films. Fabrication employs the same photolithographic process that the electronics industry uses to manufacture integrated circuits, building a device layer by layer.

Once the patterned metal layers are embedded in the flexible polymer, a tiny portion of the metal traces are exposed so they can record neural activity or stimulate brain tissue. In all, manufacturing the implants takes



Special electrochemical methods have been developed for applying polymer and metal coatings to transform the electrodes into biosensors. Photos show probes coated with the original platinum surface (center) and other biosensor-enabling coatings. Each scale bar represents 20 micrometers.

four to six weeks. The final device used in many studies consists of a polymer probe nearly as narrow as a human hair and a connector attached to the array, providing a direct, passive connection to external devices. In cases of animal use, the connector is typically secured to a headstock mounted atop the skull with a biocompatible material. For long-term human use, the researchers envision data from the implant being routed by a wireless transmitter located

elsewhere in the body, much like a heart pacemaker.

Leveraging the Artificial Retina

Haque notes that the Neurotechnology Program first gained national recognition by playing a critical role in developing the world’s first artificial retina. Also known as the “bionic eye,” this retinal prosthesis used the same biocompatible polyimides as the current brain probes and was developed for people blinded by retinitis pigmentosa or macular degeneration. Livermore engineers developed a flexible microelectrode array that conforms to the curved shape of the retina. Approved by the U.S. Food and Drug Administration (FDA) as the first high-density, microfabricated, and fully implantable neural prosthetic ever produced, the device partially restores sight to blind individuals.

The artificial retina received an R&D 100 Award in 2009 and a *Popular Mechanics* Breakthrough Award in 2010. “We are leveraging much of that retinal prosthetic endeavor,” says Haque. “The artificial retina is a great foundation from which to work.”

One of the most important features of Livermore Flexible Probes are their large number of electrodes. Whereas commercial devices commonly feature 4 electrodes, Livermore designs offer 32, 64, or even 128 electrodes. With this arrangement, a single electrode is likely to detect the activity of more than one neuron, and the activity of a single neuron could be detected by multiple electrodes. Software algorithms are often used to differentiate signals from individual neurons when the number of electrodes would make the job overwhelming for humans. “The human brain has 100 billion neurons, and a 128-electrode Livermore device can pick up activity from several hundred of the cells,” explains Haque.

Efforts are underway to increase the electrode count. Electrical engineer Angela Tooker, who is spearheading the creation of ultrahigh-density arrays, says, “Scientists would like more electrodes—1,000 per device—to record at very high densities throughout entire brain structures, such as the cortex, and across multiple brain areas.” The group’s long-term goal is to develop systems that record activity from 10,000 neurons or more to study memory, learning, addiction, and anxiety. The hippocampus, the region of the brain associated with memory, is composed of 100,000 neurons, so several high-electrode-count arrays could record approximately 1 in 10 of those cells.

Tracking Neurotransmitters

Neurons interact through both chemical and electrical signaling, but the majority of electrode arrays from Livermore and elsewhere in the neuroscience community have so far focused on monitoring only the electrical component. Livermore chemist

Anna Belle is integrating biosensors onto the standard Livermore Flexible Probe platform to understand the chemical dynamics of neuron signaling. The biosensors allow the Livermore probe to record extremely small changes in chemical concentrations in addition to electrical activity.

Current research indicates that many neurological conditions such as Parkinson’s disease, depression, PTSD, and drug addiction are related to imbalances in the production of neurotransmitters such as dopamine and serotonin. Livermore Flexible Probes are among the few tools that allow scientists to continuously measure real-time changes in neurotransmitters for extended lengths of time in ambulatory animals. By integrating chemical sensors with the probes, scientists hope to determine—first in animals and then in humans—how neurotransmitter concentrations change during various activities and compare those changes in normal brains with those of people suffering from a particular disease. Belle says, “We don’t know what an optimum level is for a lot of these neurotransmitters, but our biosensors can help establish that.”

The chemical-sensing electrodes are plated with different coatings—such as enzymes and polymers—that act like selective amplifiers to enable the targeted detection of a single chemical out of the many in a brain region. At Livermore, glutamate sensors surgically implanted into rat brains can detect very small, localized changes in glutamate

Livermore researchers are investigating the potential of implantable microelectrodes to alleviate severe depression by disrupting accompanying neural signals, an emergent treatment called deep brain stimulation. This artist’s concept depicts a variety of components that such therapy might feature, including Livermore Flexible Probes, a telemetry hub, and associated electronics. (Illustration by Kwei-Yu Chu.)

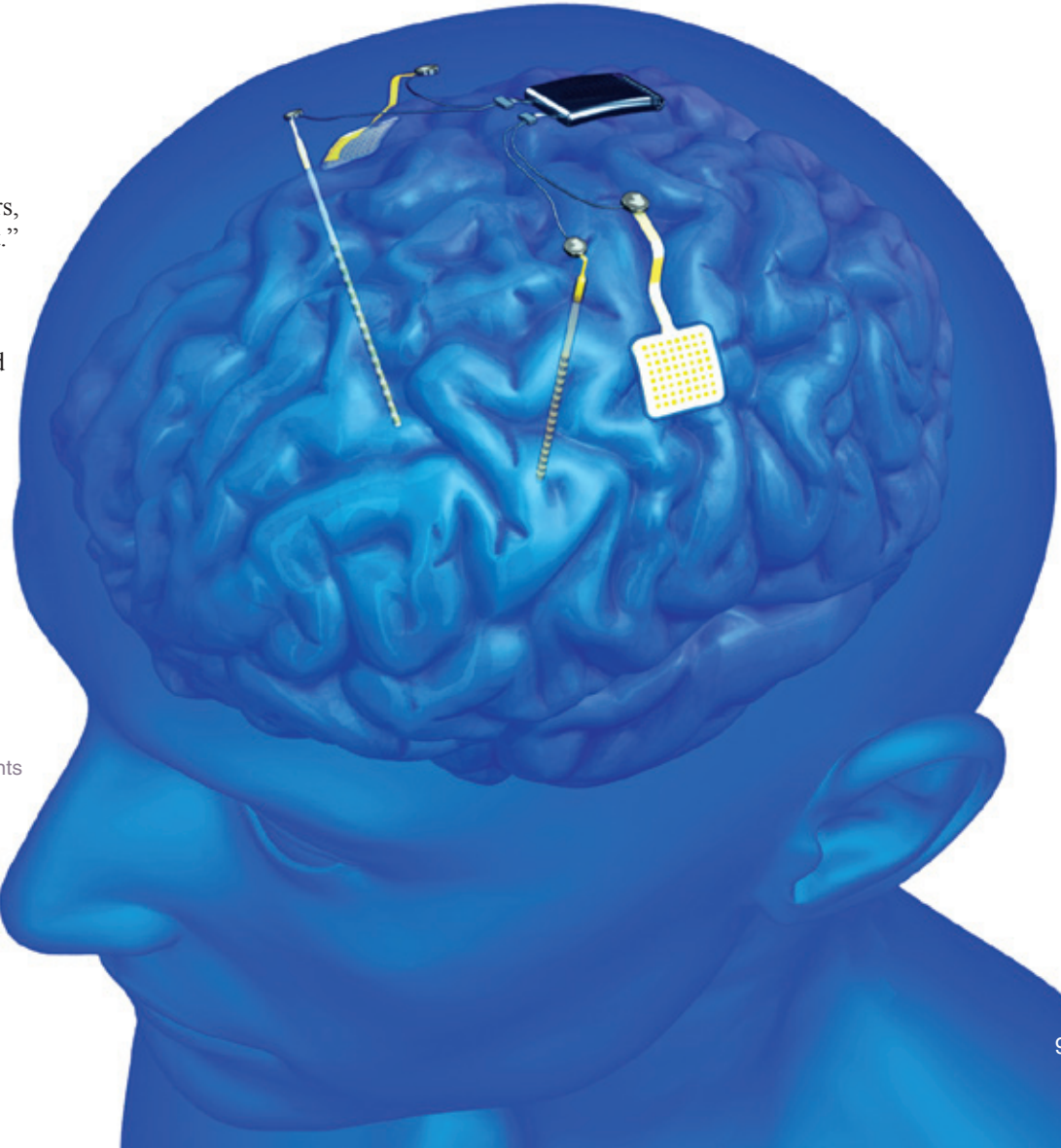
concentration as the animals move around, providing far more data than is possible with current diagnostic techniques. Such data has the potential to help researchers understand a wide range of conditions.

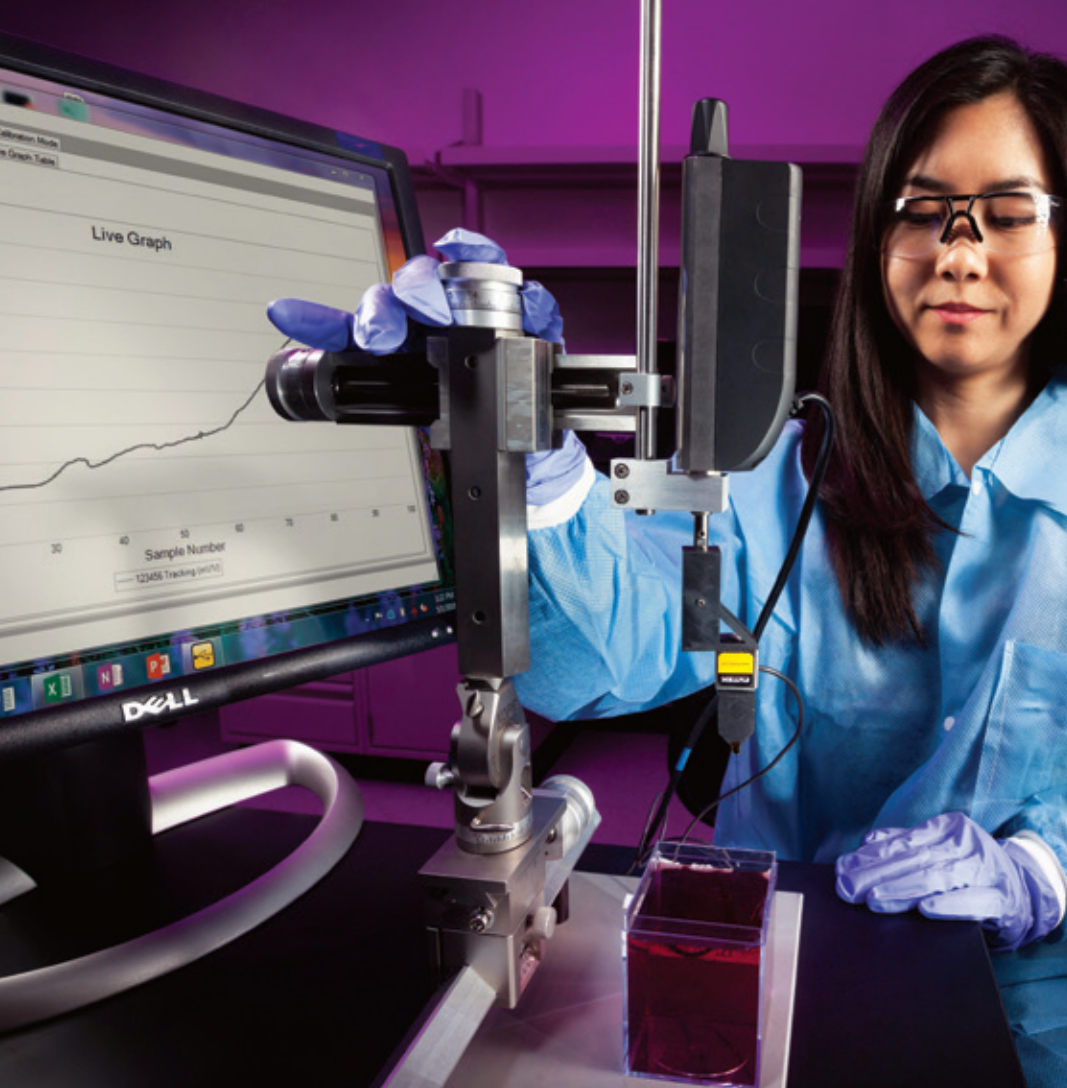
The specialized coating processes used at Livermore also allow a single probe to be equipped with multiple types of biosensors to monitor a diverse population of biomolecules simultaneously. For example, combinations of biosensors can simultaneously measure several biomarkers, including pH, oxygen, and glucose—indicators of blood flow and metabolism—and neurotransmitters such as dopamine and glutamate, which reflect normal learning and memory formation. Such biosensor combinations can also provide more information than single

biosensors can on the neural dynamics of both healthy and diseased brains. Integrating multiple biosensors onto Livermore probes will help establish optimum neurotransmitter levels and accelerate development of therapies to maintain these levels in diseased brains.

Stimulating Selected Neurons

One therapeutic use of present Livermore Flexible Probe designs is deep brain stimulation (DBS). Currently used to treat some neurological disorders such as Parkinson’s disease, essential tremor, and epilepsy, DBS is also being clinically investigated as a possible treatment for depression, neuropsychiatric disorders, PTSD, traumatic brain injury, and chronic pain, among other conditions. In DBS, surgically implanted electrical leads deliver





Researchers such as Allison Yorita can use Livermore Flexible Probes to collect an extraordinary amount of neural signaling, as seen on the monitor. (Photo by Randy Wong.)

pulses to specific brain tissue to disrupt certain electrical signals associated with the disorder.

A Livermore effort to better understand DBS and enhance its effectiveness is part of DARPA's Systems-Based Neurotechnology for Emerging Therapies (SUBNETS) program, part of the BRAIN Initiative. DARPA recognizes that surgery, medications, and psychotherapy can help to alleviate the worst effects of neurological conditions but are still imprecise and not universally effective. Through SUBNETS, the agency hopes to reach an unprecedented ability to record, analyze, and stimulate multiple brain regions for therapeutic purposes and even cure some conditions.

Haque says, "Although DBS can be used today as an FDA-approved therapy to treat Parkinson's, the current technique is imprecise, affecting broad regions of the brain, and can cause significant side effects during use." Microfabricated DBS probes could better target a brain region while avoiding unwanted effects. Haque adds, "One of the questions we are attempting to answer in support of SUBNETS is whether we can disrupt certain neural signals while someone is suffering from an episode of severe depression or PTSD. For example, we might want to search for specific electrical activity when a patient is in a particular mood state, such as severe depression, and then send a signal to a group of associated neurons to disrupt that activity." The device would be similar to a pacemaker, which is activated when the heart beats abnormally, and would not require patient intervention. Researchers in Livermore's Neurotechnology Program and

its clinical collaborators are investigating the underlying mechanisms by which DBS works to treat major depressive disorders by stimulating cells to release dopamine, for example. Haque explains, "DBS would probably not replace pharmaceuticals and would be reserved for severe cases, although data recorded by the probe could aid the development of new pharmaceuticals."

As the number of electrodes increases, the amount of information captured grows exponentially. Collaborators using Livermore Flexible Probes have helped develop an automated system called MountainSort, which sorts brain activity by individual neurons, making it possible to record and analyze unprecedented amounts of neural signals. Part of a joint project among Livermore's Neurotechnology Program, UCSF, the Simons Foundation Flatiron Institute, and Intan Technologies, the work features an algorithm and open-source software that automatically sort neural activity detected by implanted electrodes. "Current analytical approaches are time-consuming because they involve manual intervention," explains Tooker. Using Livermore's 32- and 64-channel probes, Frank's UCSF team demonstrated MountainSort's ability to collect and sort information from about 1.1 million neural events per hour. The system separated neural signals from background noise and performed better than humans manually separating these same signals, a tedious and labor-intensive process. Tooker predicts that the ability to automatically sort neural activity data at unprecedented rates will in turn drive the development of microelectrodes with higher electrode counts.

Human Use on the Horizon

By all accounts, the Livermore Flexible Probes seem ready for human use. Sundaram points out that Livermore's 128-channel probes have done exceedingly well when implanted for short periods in UCSF patients who underwent surgery

for epilepsy and who agreed to the temporary implants. During the operation, neurosurgeons recorded high-resolution electrical activity while patients responded to verbal questions. Haque explains, "The neurosurgeons said the data collected was the best they had ever seen and that recording from the hippocampus was possible for the first time." He is hopeful that the Livermore probes will be implanted in humans for longer term studies through the SUBNETS program.

"The question is how to transition from the animal to human world," says Sundaram. "Until a qualified commercial provider emerges, the Laboratory can fill the gap." He adds that Livermore's work remains unattractive to private companies because of technical challenges, high costs, a perceived small market, and the steep regulatory hurdles involved in commercially manufacturing a device for internal human use. In addition, many university groups that perform neurophysiology research on animals lack manufacturing expertise and the facilities required—such as a clean room with strict quality control standards—to extend their work from animals to humans.

Pushing the Frontiers

Sundaram states, "The Livermore team is pushing the frontiers of neurotechnology by furthering understanding of the brain and speeding development of new neurological therapies." To enable widespread adoption of Livermore Flexible Probes, the team plans to collaborate with additional laboratories in optimizing the devices and conducting studies on high-density, long-term recording. Feedback from such studies in different species and across different brain regions will provide a deeper understanding of normal and pathological brain function. Sundaram is also in discussions with NIH to designate Lawrence Livermore a national research resource center that widely distributes the Livermore Flexible Probes. At the same time, planning has begun on forming

a neuroscience consortium that brings together the Laboratory and several other institutions in the San Francisco Bay Area.

In the meantime, Livermore's Neurotechnology Program continues to progress toward the long-term goal of devices that map pathways in the brain

“The Livermore team is pushing the frontiers of neurotechnology by furthering understanding of the brain and speeding development of new neurological therapies.”

with thousands of electrodes. Researchers continue to take advantage of advances in microfabrication and new materials to develop new generations of devices with substantially increased electrode density. Tooker says, "We want to push the size limit and manufacture smaller devices with more electrodes so that each device can deliver more information." To that end, engineer and electronics packaging expert Susant Patra is leveraging Livermore's cutting-edge capabilities in lasers and manufacturing. He notes that applications inside the human body require a small, high-density package with performance that can survive the body's closed, device-unfriendly environment. One avenue of research is using Livermore's femtosecond laser to seal the components. The laser emits a pulse lasting only 50 to 1,000 femtoseconds (quadrillionths of a second)—too brief to transfer heat or shock to the materials being sealed.

Patra is investigating the use of another core Livermore manufacturing strength, additive manufacturing, in which

components are built up layer by layer according to computerized direction. Here the goal is to eschew conventional planar printed circuit boards in favor of an additively manufactured architecture that takes advantage of the third dimension—depth—to achieve the smallest possible package. Patra explains, "We want to assemble all electronics in the smallest possible form factor, with less than 500 micrometers of depth, then cover the entire device with soft materials and seal them with femtosecond lasers."

Sundaram predicts that therapies such as DBS will someday be widely adopted for the treatment of serious neurological problems. When that milestone is reached, the next step will likely be devising performance augmentation—that is, learning—techniques based on new information gleaned from implant-collected data. Such data may make possible the next human-machine interface. "Today, we have to speak or use a keyboard to communicate with a computer," says Sundaram. "Perhaps someday we will communicate using our thoughts, with a skullcap that detects neural activity and translates it to words." Haque comments, "So much about the brain still waits to be discovered. We do not even know what we are going to learn."

—Arnie Heller

DARPA approved for public release, distribution unlimited

Key Words: additive manufacturing, artificial retina, Brain Research through Advancing Innovative Neurotechnologies (BRAIN) Initiative, deep brain stimulation (DBS), Defense Advanced Research Projects Agency (DARPA), depression, epilepsy, femtosecond laser, hippocampus, implantable electrodes, Intan Technologies, Laboratory Directed Research and Development Program, Livermore Biomedical Foundry, Livermore Center for Bioengineering, Livermore Flexible Probes, MountainSort, National Institutes of Health (NIH), Parkinson's disease, post-traumatic stress disorder (PTSD), Systems-Based Neurotechnology for Emerging Therapies (SUBNETS), traumatic brain injury.

For further information contact Shivshankar Sundaram (925) 423-6468 (sundaram1@llnl.gov).

BUILDING A NETWORK OF COLLABORATIVE AUTONOMOUS MACHINES

A FIREFIGHTER enters a burning office building followed by several drones, searching for people in need of rescue. The drones scatter in different directions, moving down corridors and systematically scanning rooms. Each drone’s onboard sensors measure smoke, temperature, sound, and motion to determine which places are too hot or smoky for the firefighter to approach and which spots show signs of a living human being.

No single drone acts as a central control device. Instead, the drones in this hypothetical squadron communicate with each other and use their powerful algorithms and ample computing power to pool and process their data and decide, as a group, whether a survivor has been detected and, if not, where to continue the search. The drones also “know” enough to avoid conditions that would disable them. The firefighter receives reports from her drone squadron and can command the devices, but she has no need to control each drone’s every action—the devices have sufficient algorithmic might to operate on their own in real time, deciding collectively when their human partner needs to know about certain information. Such behavior by a group of networked devices is called collaborative autonomy, and Livermore researchers are working to make it a reality.

A human-machine firefighting team is just one example of collaborative autonomy’s potential. “Any task that is dangerous, repetitive, or dirty would benefit from this capability,” says Livermore’s Reginald Beer, the leader of the research effort. The software and hardware for collaborative autonomy could be applied not only to drones but also to mobile surface or underwater robotic vehicles, self-driving cars, and even appliances in the Internet of things—in other words, machine agents of all kinds. Devices so equipped could perform search-and-rescue operations for missing persons in a wilderness area or after a disaster, look for a hidden nuclear device by detecting its radioactive signature, or measure the movement of a hazardous chemical release and assist in containing and cleaning up the substance, to name only a few possibilities.

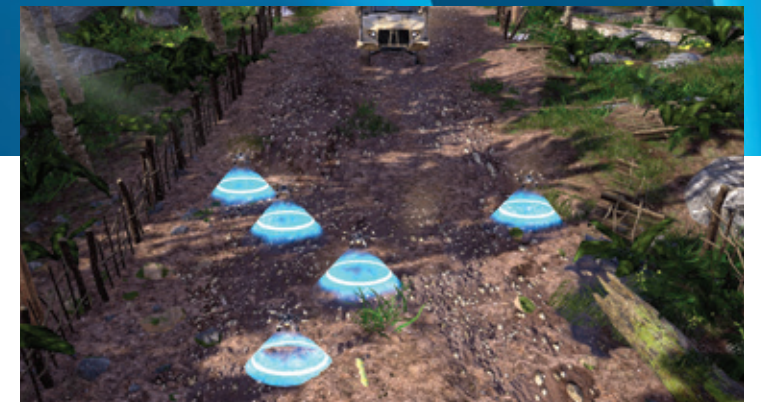
Extending the Reach of Radar

Livermore’s collaborative autonomy research is a natural outgrowth of a project to develop vehicle-mounted ground-penetrating radar (GPR) for detecting buried objects in real time. Beer’s team developed an array of radar transmitters and receivers for the effort, which has applications such as

detecting buried explosive devices. As the GPR-equipped vehicle moves forward, the array produces an image of what is located underground in a vertical plane. The system processes data much the same way that medical computerized tomography generates a planar image of the body’s interior. Beer realized that the system could be given algorithms that not merely generate an image from the data but also interpret the image and relay that interpretation to the human operator. “From there, it was a natural step to imagining a team of sensors that can test for more types of targets and could even be airborne instead of mounted on a ground vehicle,” he says. For GPR, he envisions a group of drones that fly ahead of a vehicle, autonomously select the areas on which to concentrate their scans, collaboratively interpret their data, and alert the vehicle’s operator to the presence of a buried explosive device, which the operator then disables.

In short, the ultimate goal of this collaborative autonomy research is to develop software and hardware that allows a group of machine agents to collaboratively gather sensor data (observe), identify and interpret what the sensors detect (orient), make decisions about how to respond (decide), and implement those decisions (act). Furthermore, such a system must be able to decide

Livermore researchers are using simulations to improve communications between networked machine agents, such as drones. In these screen captures from video representing such a scenario, (below) a fleet of drones supports a vehicle using ground-penetrating radar to find buried explosive devices. The drones fly ahead of the vehicle, using their sensors to detect any buried metallic objects. (top) When a buried explosive is found, the drones notify the vehicle’s human operator, who can then avoid the explosive. (Renderings by Adam Connell.)



and act quickly enough in real time to be useful to humans. In achieving the considerable technological advances required to realize this vision, the Livermore team began with the first step—developing and testing the algorithms for decentralized processing and communications in autonomous sensor networks.

Autonomy through Decentralized Computing

A project funded by the Laboratory Directed Research and Development (LDRD) Program and led by computation engineer Ryan Goldhahn focuses on creating decentralized processing and communications algorithms, while partners at the University of Texas at Austin are developing hardware for algorithm testing. Goldhahn says, “We wanted to move away from the model of nodes sending data to a central command center. That model is not scalable because of the vast amounts of data that must be centrally processed. In addition, the central node—such as an autonomous vehicle, a computing cluster at a command center, or any other type of lone machine agent—is a vulnerability because if the central node fails so does the entire network.” With recent technological advances allowing engineers to equip each individual node with considerable processing power, the project team is working on a real-time capability in which each member of a large network possesses a high degree of autonomy.

Goldhahn explains, “Each node must be able to decide which data matter and communicate those data to the rest of the network. We are using what are called gossip and consensus algorithms, in which one node sends a measurement deemed

relevant to its neighboring nodes. As they exchange more and more data, the nodes agree on what they are sensing.” The algorithms also eliminate the problem of “Byzantine data”—poor measurements or deliberate misinformation—by first agreeing what data are significant and then deciding where additional measurements are needed to be more certain of their interpretation. One capability required for such a system is determining which nodes in the group will make the subsequent measurements and which nodes will relay those measurements to the rest of the group. To this end, each node must autonomously decide where to position itself relative to the other nodes and whether to investigate a potentially important event. The entire group must agree on who does what without any one node being in overall command. A significant challenge is to achieve a decision making capability that can be scaled up to hundreds of nodes without overwhelming the network with computational complexity or communications volume.

Simulating Network Communication

An important aspect of this effort is to achieve maximum efficiency in communication among the nodes. To this end, the researchers are studying simulations of sensor networks run on Livermore’s high-performance computing resources. Computer scientist Peter Barnes leads Livermore’s network simulations team, which has developed the capability to simulate realistic networks—on the order of 10,000 to 500 million computers—using the open-source software program ns-3.

Barnes and Anton Yen are developing the ability to computationally model communications and other behavior among nodes using a simulated set of nodes. “Communications technology faces constraints on bandwidth and range, such as the time it takes for information to travel,” says Barnes. “In addition, a specific node may need to communicate only to one other node but not all the others, or may send and receive messages to and from multiple nodes nearby.” The simulations are therefore examining internodal communications in great detail, from parameters such as range, latency, and bit rate to the impact that the parameters have on the collaborative autonomy algorithms. The ultimate goal is to optimize the process of gathering, sharing, and interpreting the data and calculating the next steps.

A Belief Network

Gerald Friedland, a computation scientist at Livermore and an adjunct professor at the University of California at Berkeley, is leading an LDRD project to apply Bayesian belief propagation to collaborative autonomy. Specifically, Friedland and his collaborators Kannan Ramchandran and Maya Gokhale are developing software and hardware for a network that uses Bayesian statistics to arrive at a belief, that is, to compute the



Lawrence Livermore collaborators at the University of Texas at Austin have developed this drone prototype along with a network simulation platform. Together, the hardware and software test the ability of individual nodes in a mobile network to collect and share sensor data.

In this network simulation, a fleet of machine agents—drones or other devices—is deployed to detect targets. Individual agents communicate with others nearby but not necessarily with every agent in the fleet. Gossip and consensus algorithms allow the agents to (top) share sensor data about possible targets and (bottom) arrive at a consensus about a likely target.

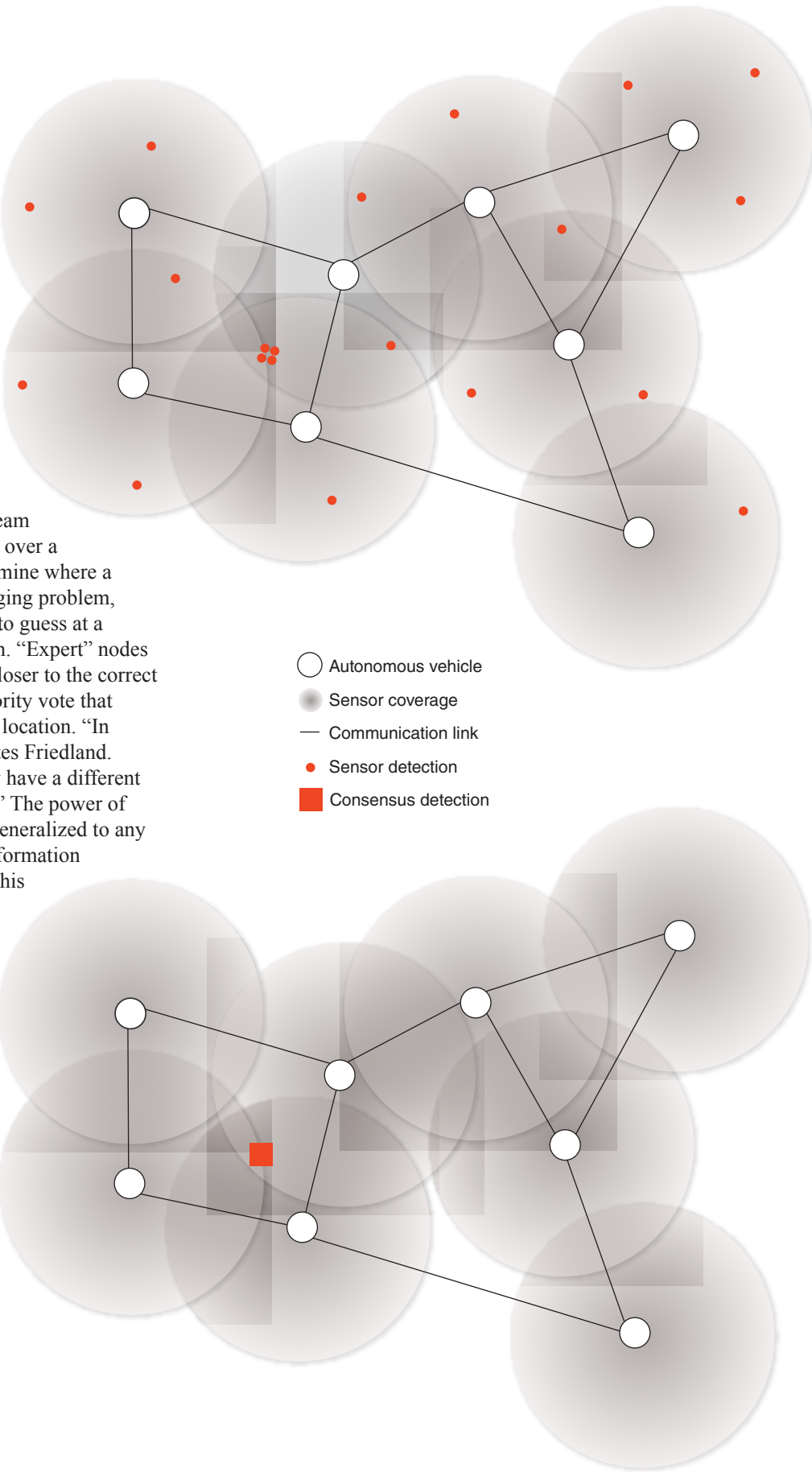
probability of a particular outcome. For instance, as each node in the network collects data from its sensors, the nodes “vote” to arrive at a consensus interpretation of the data.

Using YFCC100M—an open-access database of more than 100 million photos and videos for artificial intelligence research—the team is developing algorithms that will be distributed over a network so that the nodes can collectively determine where a specific video was filmed. To solve this challenging problem, nodes will use visual, audio, and even text data to guess at a location and then vote repeatedly on the location. “Expert” nodes will emerge from the group by virtue of being closer to the correct answer than others, leading eventually to a majority vote that represents a collective consensus on the video’s location. “In some ways, the nodes behave like humans,” states Friedland. “One node has a certain belief, and another may have a different belief, and the two nodes can agree or disagree.” The power of the belief-network approach is its ability to be generalized to any problem, exploiting and combining available information to arrive at the best possible answer. As part of this LDRD project, Friedland’s team will install the software in specially developed hardware—field-programmable gate arrays designed to be lightweight, fast, and low power. These collaborative autonomy efforts are joining forces to take the first steps toward what Beer calls a “networked machine intelligence that is capable of autonomy of action.”

—Allan Chen

Key Words: Bayesian network, belief network, byzantine data, collaborative autonomy, consensus algorithm, decentralized processing, field-programmable gate array, gossip algorithm, ground-penetrating radar (GPR), Laboratory Directed Research and Development (LDRD) Program, network simulation, node, ns-3, sensor network, YFCC100M.

For further information, contact Reginald Beer, (925) 424-2232 (beer2@llnl.gov).

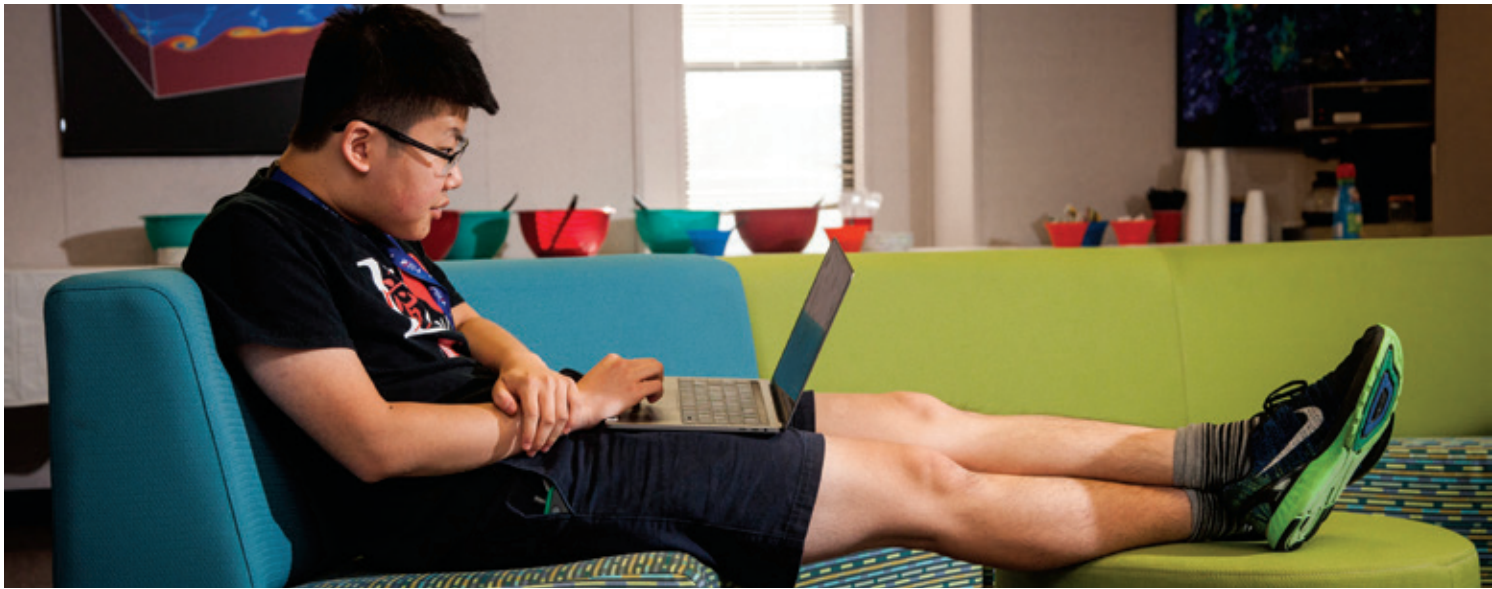


GRASSROOTS INNOVATION GROWS GREAT COMPUTATIONAL IDEAS

THE Computation Directorate at Lawrence Livermore provides researchers with the cutting-edge hardware and software needed to conduct potentially world-changing work in the Laboratory’s mission space. Capabilities range from web application development to some of the most powerful computers on the planet, all driven by innovation aimed at benefitting the nation. One way Computation sustains technical leadership is by innovating for itself—investing in the people and ideas that will support Livermore’s pioneering work today and tomorrow.

Harnessing the special skills of its software engineers, developers, programmers, and system administrators, Computation has adopted a novel set of programs designed to foster worthwhile concepts and see them to their logical conclusions. Developer Day, Hackathon, and Idea Days can take a programmer’s innovative idea and help her determine how to put that idea to work.

Development groups from various Laboratory organizations gathered together in September 2017 for the first Developer Day, where ideas and solutions could be shared across the Laboratory. Feedback was overwhelmingly positive, and another Developer Day is being planned for summer 2018. (Photos by Randy Wong and Lanie Helms.)



Diving into the Talent Pool

Lawrence Livermore employs close to 8,000 people. Some are dedicated to operating the world’s most powerful laser while others model complex systems on supercomputers and still others work to advance global security, to name just a few. Each effort, along with the rest of Livermore’s programs and operations, requires some degree of Computation’s support. To meet the specific needs of each Livermore organization, many Computation employees are assigned—or “matrixed”—to organizations all across the Laboratory. While allowing Computation employees to focus on their customers’ needs, this arrangement can also make it difficult for geographically scattered Computation employees to get together and share ideas. “The matrix approach is good for Livermore programs because it allows them to pull from the large pool of Labwide talent,” says Kyle Dickerson, a web application developer matrixed to the Global Security Directorate. “But a side effect is that a matrixed person might not be interacting very frequently with other people of the same specialty.”

Developer Day brings together the Laboratory’s software community to improve productivity and sustainability, amplify useful software practices, and promote shared practices. Dickerson was a member of the event’s inaugural organizing team, which also



“Hackathon was the perfect place to try to see whether the technology would succeed or fail.”

included David Beckingsale, Todd Gamblin, and Cyrus Harrison. Their plan was to jump-start communication among different programs doing similar work. Dickerson states, “The programs have a lot of common frameworks, programming languages, tools, and work environments. Many of us are also solving common problems, so if one of us solves a problem, it would be more efficient for the Laboratory if another group did not have to solve that same problem all over again.”

Avoiding unnecessary repetition is a large part of what made the first Developer Day a huge success in September 2017. The day began with a series of “lightning talks”—five-minute presentations that development teams from around the Laboratory gave about their work and the languages, frameworks, and platforms they use. These short introductions also helped bridge the information gap and inform attendees about other opportunities throughout the Laboratory. After the lightning talks, the organizers encouraged participants to strike up conversations during short breaks and further explore the efforts of their colleagues. Longer talks focused on hiring and onboarding the right candidates, along with “deep dives” into special programming concerns at Livermore—such as how to synchronize code and data across an air-gapped network—that cannot be solved with standard industry approaches. The feedback, Dickerson says, was overwhelmingly positive. In a 2017 survey, 100 percent of respondents said they hoped the event would be held yearly, and plans are already underway to bring Developer Day back in the summer of 2018.

Sharing ideas and collaborating can have concrete results. Dickerson remembers one attendee realizing that his next project might not take eight months as he had thought. “He said, ‘If I just talk to two groups at the Laboratory, I can probably get it done in a month instead.’ Those groups had already solved all the issues he was facing,” says Dickerson. “Developer Day is just one day of attendees’ time. If, because of it, a project takes one month instead of eight, that is a win.”

Hacking It

Big wins in productivity can lead to even bigger ideas. To this end, Computation several years ago launched Hackathon (see *S&TR*, June 2003, pp. 16–18). The event is described as “a 24-hour chance to brainstorm, foster creativity, learn new

things, accomplish something fun that might not be on the top of a developer’s to-do list, build prototypes, and explore something new—even if it fails.” Gary Laguna, a computer scientist supporting Livermore’s Environmental Protection Department, sits on Hackathon’s steering committee. He explains, “What often happens is that someone at Hackathon uses the time to flesh out an idea they’ve been thinking about but never had the time to work on in their day-to-day responsibilities. Hackathon gives people a chunk of time to try out an idea and see whether it works.”

For Justin Barno, a developer in Global Security’s geophysical modeling program, interest in Hackathon began as a way of learning Spark, a new Java interface that could help solve some of his group’s data challenges. The challenges were not immediately urgent, but he knew they would be someday soon. “Whether it was Spark or another technology, we needed something,” says Barno. “Hackathon was the perfect place to see whether the technology would succeed or fail, or whether it was even useful in the first place.” Today Barno is a member of the organizing committee tasked with evolving



Computation’s thrice-annual Hackathon invites participants from all over Lawrence Livermore to work on any project that may benefit their work in the short or long term. Organizers say the 24-hour timeframe encourages people to “fail fast” and learn a lesson, then move on to the next idea. (Photo by Randy Wong.)

the thrice-yearly event—and keeping the coolers full of soda. The atmosphere that allows participants to “fail fast” comes, Laguna says, from its grassroots organizational structure—or relative lack thereof. “We have a really good recipe right now,” he adds. “I would be hesitant to put too much structure into the event.”

For Robert Blake, Yuriy Ayzman, and Shivshankar Sundaram, the spring 2017 Hackathon was an opportunity to experiment with how magnetic resonance images of the human heart are processed. Usually, doctors have to painstakingly separate the heart from the rest of the picture, pixel by pixel. However, by the end of the 24-hour Hackathon, the three had determined how to use neural networks to understand test images better and produce results that rivaled those of existing tools. In short, their Hackathon-inspired idea yielded an innovation with much promise.

The Next Step

For successes such as those achieved at Hackathon, Computation also provides a funding source that supports the most promising projects into their next stage of evolution. During a twice-yearly event called Idea Days, any Computation employee can propose an idea to a committee of colleagues and, if the idea is accepted, receive up to two full weeks of funding. Proposals are informal, short, and known only to the committee until the selected projects are published. Idea Days does not fund actual research but rather supports projects meant to benefit Computation and the Laboratory more broadly. In May 2017, one such proposal came from Ayzman, Blake, and Sundaram’s team, hoping to build on their Hackathon project and further automate cardiac image processing. The three proposed enhancing deep-learning models in a way that would greatly benefit machine-learning efforts across the Laboratory, in addition to making image processing in general more efficient and robust.

A subset of proposals are selected for “Pitch Day,” where employees explain their idea in detail—the problem to be solved, how to solve it, and the benefits expected. When a funded project is completed, the team is required to report back to the committee on the results achieved. The entire process is designed to be fluid, uncomplicated, and unrestricted so as not to impede creativity or originality. Ayzman, Blake, and Sundaram were successful with their Idea Days application. The project was so successful, in fact, that further funding was approved by Katie Lewis, head of Computation’s Applications, Simulations, and Quality Division. Today, the team is using its image-processing automation approach to improve data analysis at the National Ignition Facility, the world’s most powerful laser and the site of important experiments in stockpile stewardship.

Idea Days, Hackathons, and Developer Days together form a mechanism that allows software engineers, application developers, web designers, and a host of other Computation employees to smoothly and efficiently pioneer improvements



Cyrus Harrison, a Developer Day organizer, Livermore computer scientist, and associate division leader, explains his work in the Applications, Simulations, and Quality Division during a “deep dive,” a talk that delves into a specific issue or endeavor. (Photo by Lanie Helms.)

that better enable the entire Laboratory to deliver on its missions. By thus cultivating new ideas from all aspects of the Computation Directorate, the Laboratory is equipping itself with the technological know-how that will be needed for the next generation of research—and researchers.

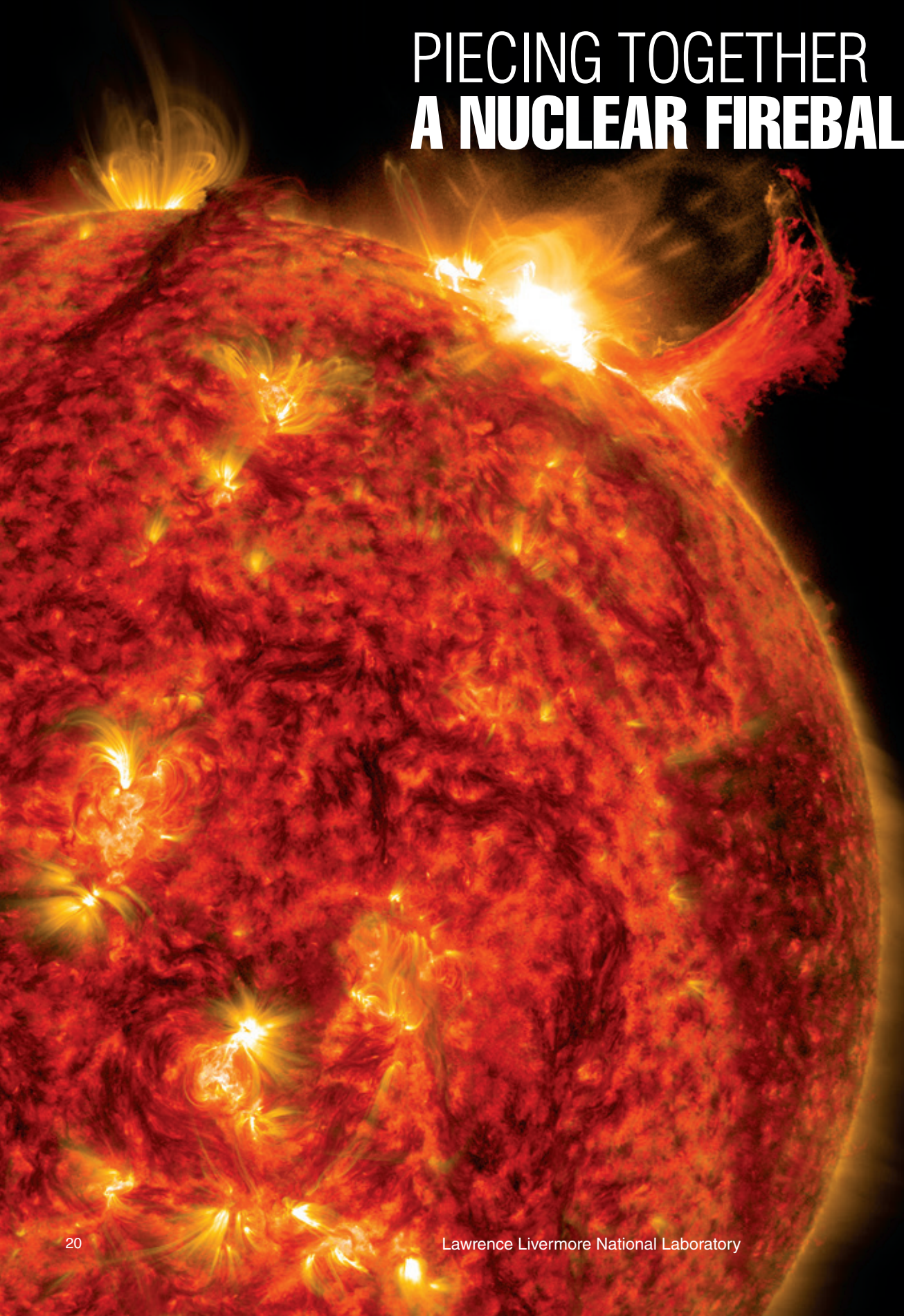
“My belief is that the people who are drawn to events like these are the people who will truly be the drivers at the Laboratory in the future,” says Laguna. “They are the ones who want to do things beyond their day-to-day jobs. They want to push the envelope and try new things. That is something the Laboratory and the nation will always need.”

—Ben Kennedy

Key Words: application development, Computation Directorate, Developer Day, Hackathon, Idea Days, innovation, image processing, web development.

For further information contact Lori Diachin (925) 422-7130 (diachin2@llnl.gov).

PIECING TOGETHER A NUCLEAR FIREBALL



Resulting from the Sun's nuclear processes, the erupting plasma from solar flares rapidly expands and cools similarly to what occurs in a nuclear fireball. (Image courtesy of NASA/SDO.)

MATERIALS vaporized by a nuclear explosion do not simply disappear without a trace in the resulting fireball. Leftover bomb materials and fission products remain, but these interact with the surrounding environment in complicated ways, making it difficult for scientists to unravel what happened in the explosion. However, by better understanding the chemical compounds that form in the cooling fireball, researchers can more effectively uncover evidence that can help identify the nature of the bomb that produced the blast. In the event of a nightmare scenario such as the detonation of a nuclear weapon in a U.S. city by a rogue actor, such forensic capabilities would be invaluable.

The tremendous energy generated by a nuclear explosion instantly vaporizes any nearby materials. On an atomic level, electrons are stripped away from gaseous atoms to form a plasma—a mix of ions from different elements and free electrons. As it rapidly expands, the plasma quickly cools back into gases, liquids, and finally solids. During this sequence of phase transformations, the different elements segregate according to their chemical properties and fractionate (that is, separate out) as they condense into solids, forming the particles known as fallout debris. All this begins to happen within moments after the explosion, once the temperature drops below roughly 5,000 kelvins and the pressure has subsided to approximately atmospheric level.

The ability to disentangle the effects of this fractionation process is essential for accurately piecing together a nuclear fireball. To study this complex fractionation process, researchers at Lawrence Livermore and collaborators from Stanford University and the University of Illinois at Urbana-Champaign (UIUC) have developed two different methods of physically simulating the plasma conditions in nuclear fireballs: pulsed laser ablation and the plasma flow reactor method. Research with the latter method is headed by Livermore radiochemist Tim Rose. “An advantage of having both methods running in parallel is that we cover two timescales, which differ by three orders of magnitude,” says Rose. “Pulsed laser ablation heats and cools very rapidly, in microseconds. However, events in a plasma flow reactor happen over tens of milliseconds, even as slowly as a tenth of a second.”

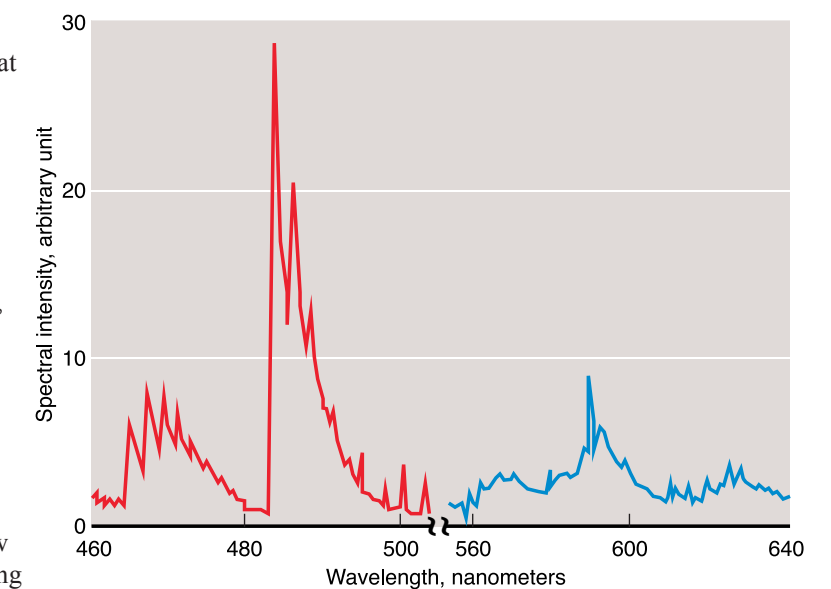
Plasma Flow Reactor Experiments

Starting as a project funded by the Laboratory Directed Research and Development Program, work with the plasma flow reactor method initially focused on one element at a time, looking at how each reacts with oxygen. Iron was examined early on as an element commonly found in debris and one that follows a straightforward pathway when forming chemical compounds.

A plasma flow reactor is an open-ended quartz tube, 1 meter in length and 4 centimeters in diameter, with a radiofrequency induction coil at one end. The coil forms a plasma torch that

heats a constant inward flow of inert argon into a plasma. Dissolved in a nitrate solution, iron is atomized and injected into the plasma torch, the hottest part of the reactor. Livermore postdoctoral researcher Batikan Koroglu explains, “The end-to-end temperature profile along the tube is well constrained, steeply decreasing from 5,000 to 1,000 kelvins. The reactor operates in steady state, so that the setup is like a nuclear fireball frozen at a moment in time.” After physically mixing with the stream of plasma, the iron ionizes, then cools while flowing down the reactor tube and begins to react with oxygen to form individual molecules of iron oxide (FeO). These molecules condense into a liquid, which finally solidifies into FeO particles.

By probing various positions along the tube in situ, optical emission spectroscopy reveals where the FeO chemically forms. This information in turn indicates at what temperature the reaction occurs. Inserted into the cooler end of the tube, a sample collector captures particles at different positions, thereby sampling different temperatures. Captured particles are analyzed using electron microscopy to uncover their morphology and microstructure. After iron, the researchers separately studied aluminum and uranium, also common constituents of nuclear debris. Once these individual metals had been looked at, combinations of metals were then evaluated.



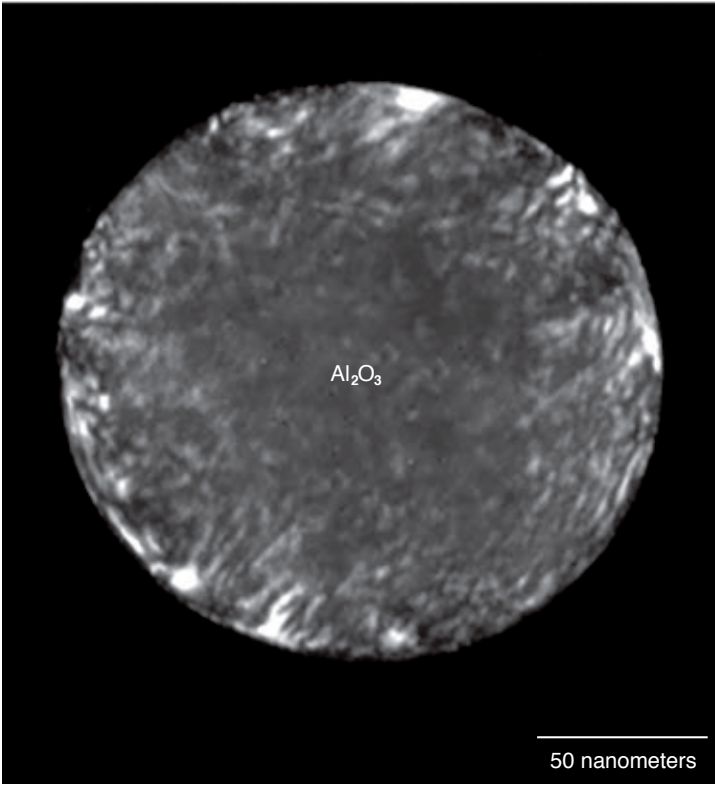
In experiments simulating conditions in a nuclear fireball, equal amounts of iron and aluminum were injected into a plasma flow reactor. The patterns of emission spectra, like separate sets of fingerprints, reveal the presence of both aluminum oxide (red) and iron oxide (blue) in gas at 1,740 kelvins that cooled from plasma.

Rose adds, “The oxide particles of uranium look different than those of aluminum, which look different than those of iron. Experimenting with multiple metals together results in even more complexity. For instance, an aluminum oxide particle that formed early in the process may have iron oxide particles sticking to it, indicating that the aluminum oxide condensed first.” Investigating the interrelation between metals provides more clues that researchers hope will lead to a better understanding of chemical fractionation inside a fireball.

Plasma by Pulsed Laser Ablation

Livermore physicist Harry Radousky, who leads the pulsed laser ablation work at Livermore, states, “Laser ablation is much

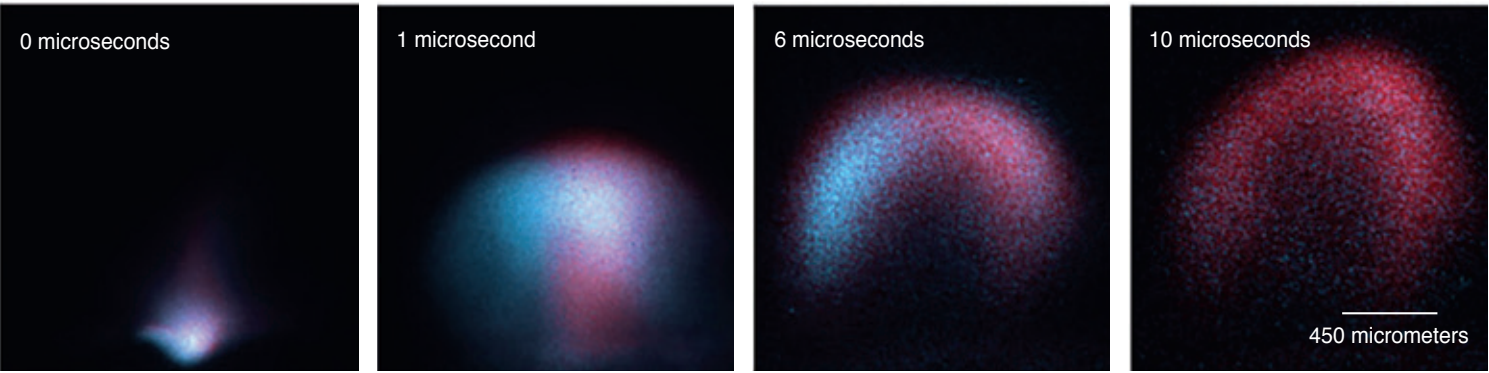
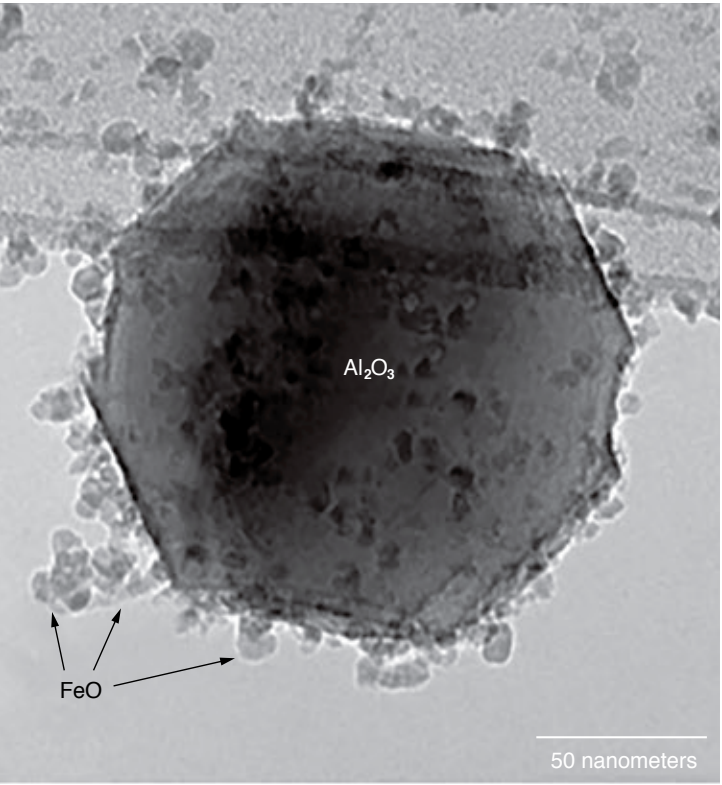
(left) Collected at a location of 16 centimeters downstream from the radio-frequency coil of a plasma flow reactor, the aluminum oxide (Al₂O₃) particle shown in this transmission electron microscope image is a perfectly spherical, single-crystal condensate. (right) A similar image shows the results of an experiment conducted with both iron and aluminum together. The large Al₂O₃ particle, which condensed early in the cooling process, is surrounded by small traces of more volatile iron oxide particles (FeO), which condensed later.



different than the plasma flow reactor method in that it is not steady state. Instead, the method involves creating a plume of plasma that changes very rapidly in temperature and density. In addition, we can carefully control the surrounding atmosphere that interacts with the plasma.” Radousky, chemist David Weisz, and physicist Jonathan Crowhurst run the experimental aspects of this research at Lawrence Livermore while collaborators at UIUC conduct the kinetics modeling.

The team recently studied strontium and zirconium, both of which are fission products created after a nuclear detonation. As with the metals studied with the plasma flow reactor, strontium and zirconium undergo the same change in state—from plasma to gas, gas to liquid, and finally liquid to solid. To compare the dynamic behavior of these elements as they condense, the researchers use strontium zirconate (SrZrO₃), an oxide with a uniform distribution of strontium and zirconium throughout its lattice. A crystal of SrZrO₃ is mounted inside the reactor’s sealed sample chamber. A beam is fired from a neodymium-doped yttrium–aluminum–garnet laser, entering the chamber and breaking down the crystal’s surface layers into ions, which erupt as a plume of plasma initially at a temperature of approximately 10,000 kelvins.

Optical emission spectroscopy is again used to analyze the chemicals that form as the plasma cools. Filters reveal the



spatial distribution of strontium oxide (SrO) and zirconium oxide (ZrO) as the plasma evolves over time. Researchers found that ZrO—a precursor to ZrO₂—formed sooner than SrO in the vapor, which was consistent with their thermodynamic properties. In short, the stable and highly refractory oxide ZrO₂ can exist as a solid at higher temperatures, and may condense earlier, than SrO. Weisz adds, “We then took the experiments one step further and demonstrated that the earliest ZrO formed from reaction with oxygen released by the SrZrO₃ crystal, whereas later ZrO formed by reaction with gas in the surrounding environment.” These reactions were verified by conducting ablation with the sample chamber filled with oxygen-18, a rare but stable oxygen isotope. Because SrZrO₃ is naturally rich in the more common isotope of oxygen (oxygen-16), the isotopic shift exhibited by oxygen-18 in the ZrO was easy to detect in its emission spectrum.

This oxygen-scavenging behavior yields insight into how early-forming oxides could reduce the amount of oxygen available for other types of compounds to form as the plasma cools. Laser ablation experiments were conducted with uranium, one of the key elements used in fission nuclear weapons. Again, two oxygen isotopes were used in the experiments to confirm the resulting uranium oxide’s stoichiometry (the numerical relationship of elements and compounds as reactants and products in a chemical reaction). As with the plasma flow reactor work, further understanding also leads to experiments of greater complexity.

Where the Forensics Lead

In an idealized nuclear airburst occurring high above the ground, the resulting fireball interacts only with air and bomb materials, resulting in debris consisting of relatively known and homogenous materials. However, the fireball from a detonation near, at, or below the surface will consume materials from the ground. Some of these materials will vaporize while others—especially in the fireball’s late stages—will remain solid. Rose says, “A debris sample picked up from the ground after detonation will represent not the initial composition of the

A plume created by pulsed laser ablation erupts from a strontium zirconate crystal over a timeframe of 10 microseconds. The formation of zirconium oxide (blue) dominates the emission spectra early on, followed by the formation of strontium oxide (red).

fireball but rather what condensed out of the fireball at certain points in its evolution.”

As they better understand how individual debris components fractionate, the researchers have added more components to their experimental mixtures. This growing complexity better represents real-world scenarios and makes their experiments and the results increasingly accurate. In the future, researchers aim to study more components mixed together in a plasma, including silica and other carrier materials that might enter the fireball from the ground and remain solid. Eventually, this work will lead to a comprehensive understanding of the basic science behind chemical fractionation that is needed to create predictive models. Validated by both modern experimental data and historic empirical data, such models would prove invaluable not only to nuclear forensics investigators but also to those monitoring the consequences of a nuclear explosion.

“These models will allow us to examine matrices that are not necessarily represented in our test history,” explains Rose. “We could simulate an urbanlike matrix and see how the condensation patterns are affected, including whether the results match our predictions. This understanding of fractionation and debris formation would be extremely helpful if we ever have to collect debris after an unthinkable event.”

—Dan Linehan

Key Words: chemical fractionation, electron spectroscopy, fireball, fission, forensics, fusion, nuclear explosion, Laboratory Directed Research and Development Program, optical emission spectroscopy, oxide, plasma, plasma flow reactor, pulsed laser ablation, uranium.

For further information contact Tim Rose (925) 422-6611 (rose23@llnl.gov).

In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory. For the full text of a patent, enter the seven-digit number in the search box at the U.S. Patent and Trademark Office’s website (<http://www.uspto.gov>).

Patents

Detector and Related Devices, Methods and Systems

Jane P. Bearinger
U.S. Patent 9,804,151 B2
October 31, 2017

Systems for Production of Polymer Encapsulated Solids

William L. Bourcier, Roger D. Aines, Sarah E. Baker, Eric B. Duoss, Amitesh Maiti, Jeffery J. Roberts, Christopher M. Spadaccini, Joshua K. Stolaroff, John J. Vericella, Jennifer A. Lewis, James O. Hardin, IV, William C. Floyd, III
U.S. Patent 9,821,287 B2
November 21, 2017

Chip-Based Droplet Sorting

Neil Reginald Beer, Abraham Lee, Andrew Hatch
U.S. Patent 9,822,403 B2
November 21, 2017

Crystalline Boron Nitride Aerogels

Alexander K. Zettl, Michael Rousseas, Anna P. Goldstein, William Mickelson, Marcus A. Worsley, Leta Woo
U.S. Patent 9,840,414 B2
December 12, 2017

Ultra Low Density Biodegradable Shape Memory Polymer Foams with Tunable Physical Properties

Pooja Singhal, Thomas S. Wilson, Elizabeth Cosgriff-Hernandez, Duncan J. Maitland
U.S. Patent 9,840,577 B2
December 12, 2017

Nanoporous Metal–Carbon Composite

Marcus A. Worsley, Joe Satcher, Sergei Kucheyev, Supakit Charnvanichborikarn, Jeffrey Colvin, Thomas Felter, Sangil Kim, Matthew Merrill, Christine Orme
U.S. Patent 9,844,762 B2
December 19, 2017

Awards

Three Lawrence Livermore scientists—**Nathan Barton**, Laboratory Director **William Goldstein**, and **Robert Kirkwood**—have been selected as 2017 **fellows** of the **American Physical Society** (APS). Election to APS fellowship recognizes exceptional contributions to the field of physics through research, leadership, applications of physics, or contributions to physics education. APS fellowship is considered a distinct, prestigious honor because members are nominated and elected by their peers, and the number of APS fellows elected each year is limited to no more than one-half of one percent of the membership.

Barton, currently head of Livermore’s Materials Modeling and Simulation Group, was nominated by the APS Division of Computational Physics for “diverse contributions in computational materials science in support of national security interests, especially related to novel-state variable descriptions for material response under both static and dynamic conditions.”

Director Goldstein was nominated by the Division of Plasma Physics for “leadership at the Lawrence Livermore National Laboratory with high levels of integrity, scientific judgment, and national impact and for pioneering research in the theory of atomic processes in high-temperature plasmas, with applications to fusion energy, astrophysics and x-ray lasers.” Goldstein is the 12th director of the Laboratory and has more than 29 years of experience at Lawrence Livermore.

Physicist Kirkwood was selected by the Division of Plasma Physics for “exceptional experimental work demonstrating the importance of energy transfer between laser beams in plasmas, and subsequent intellectual leadership of the effort to develop a two-color option on the National Ignition Facility laser that is important for achieving symmetric implosions.”

Bey Vrancken, a Lawrence Fellow at the Laboratory, was presented by the **European Powder Metallurgy Association** (EPMA) with a **Powder Metallurgy Thesis Competition Award** in the doctorate category for his Ph.D. thesis. The thesis—*A Study of Residual Stresses in Selective Laser Melting*—details his work characterizing the residual stress distribution of selective laser melting process and correlating it with anisotropic mechanical behavior of an additively manufactured part. The award was presented at the EuroPM2017 Congress, an annual meeting on powder metallurgy in Europe. Vrancken is in the first year of a three-year Lawrence Fellowship, a highly competitive postdoctoral position awarded to candidates with exceptional talent, scientific track records, and potential for significant achievements.

Lawrence Livermore researchers were among two groups recognized by **HPCWire** with an **Editor’s Choice Award** for their work in applying high-performance computing (HPC) to solve complex challenges. The awards were presented at the supercomputing conference SC17.

Laboratory scientists involved in a partnership between the Department of Energy national laboratories and the National Cancer Institute were recognized with an award for Best Use of Artificial Intelligence for their work on CANDLE (Cancer Distributed Learning Environment), a project focused on applying machine learning to personalized cancer medicine.

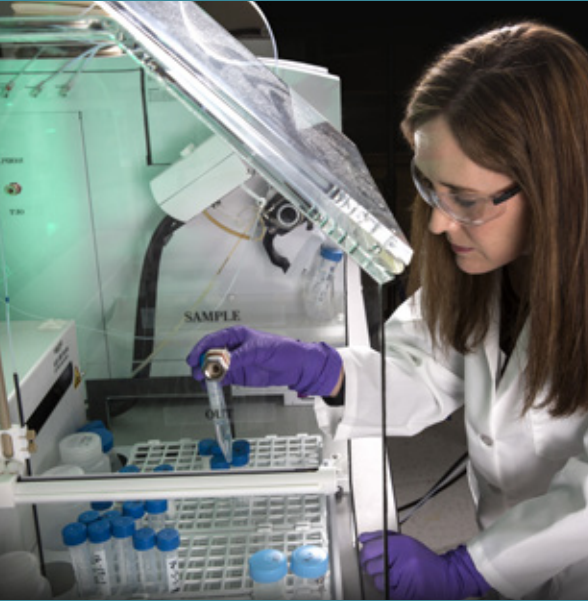
Livermore researchers garnered another prize for Best Use of HPC in Manufacturing in recognition of HPC4Mfg, a collaboration with Lawrence Berkeley National Laboratory aimed at using advanced simulation and modeling to help paper companies cut papermaking costs and energy usage. The complex models developed for HPC4Mfg targeted wet pressing, a stage in the paper-manufacturing process where water is removed from wood pulp before drying.

Delving Deeply into the Brain’s Mysteries

Lawrence Livermore’s Neurotechnology Program is designing and building extremely small, biocompatible devices called microelectrode arrays that can be implanted in the brain. These arrays, called Livermore Flexible Probes, monitor and optionally stimulate neural activity. Soft and flexible, the probes do not interfere with normal brain functions or behavior, allowing for long-term studies of brain circuitry. In research laboratories across the nation, scientists have been using Livermore Flexible Probes for recording neural activity in the brains of animals and humans. By providing high-quality, long-term, and continuous recordings of brain activity with high resolution, this Livermore work enhances a larger national effort to revolutionize understanding of the brain and uncover ways to diagnose, treat, and prevent brain disorders. Researchers are hopeful the vast amounts of data collected from the arrays will point the way to innovative treatments for both neurological disorders such as Parkinson’s disease and neuropsychiatric conditions such as generalized anxiety, depression, and post-traumatic stress disorder. In addition, the arrays may one day help to restore lost neural functions—including sight, hearing, and mobility—and reveal how people remember and learn.

Contact: Shivshankar Sundaram (925) 423-6468 (sundaram1@llnl.gov).

A Center for Cutting-Edge Forensics



With expertise in chemical, biological, radiological, nuclear, explosive, and traditional forensic analyses, Livermore’s Forensic Science Center is prepared for anything that comes through its doors—from anywhere in the world.

Also in July/August

• *Postdoctoral researchers at the Laboratory show their creativity, innovation, and expertise at the annual Research Slam.*

• *Livermore researchers have developed an algorithm that works in tandem with scientific applications to save calculation time and use high-performance computing resources more efficiently.*

• *Double-pulse x-ray technology allows researchers to study important phenomena related to nuclear weapons, including implosion and hydrodynamic stress.*

Science & Technology Review
Lawrence Livermore National Laboratory
P.O. Box 808, L-664
Livermore, California 94551

PRSRT STD
U.S. POSTAGE
PAID
San Bernardino, CA
PERMIT NO. 3330



Printed on recycled paper.